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13. ABSTRACT (Maximum 200 words) Two computational techniques have been developed to model heterogeneous and non-equilibrium phenomena in reactive inorganic mixtures under high pressure shock wave loading. The first, known by its acronym VIR, is based on a continuum mixture theory and focused on modeling the interaction between chemical reaction and hydrodynamic flow. The second is a new computational tool called DM2 and is based on a discrete element approach. The second is primarily concerned with modeling of complex interactions of thermal, mechanical, and chemical processes at the particle level on the order of micrometers. Significant findings from numerical experiments by use of these techniques include (1) a demonstration of condensed phase detonation, (2) a mechanistic description of shock-induced chemical reactions at the particle level, (3) a model demonstration of thermal explosion in shear bands, and (4) a confirmation of new deformation and failure response of metals under high-pressure shock compression.				
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INTERACTION OF SHOCK WAVES WITH MATERIALS HAVING
ENGINEERED REACTIVE MICROSTRUCTURES

FINAL PROGRESS REPORT

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I. INTRODUCTION

High-pressure shock compression chemistry of inorganic solids has been of interest for two reasons. The first is materials synthesis exemplified by the synthesis of diamond and other ultra-hard materials. This line of research has been well established since the 50's. The second, more recent interest, is based on observations of unusual chemical reactions in powder mixtures such as Ni+Al, Ti+Si, and Al+Fe₂O₃ and their potential as a new class of energetic materials whose energy release is thought to involve mechanisms that are different from those of conventional energetic materials.

The primary focus of our research project has been the second category aimed at development of computational techniques to model a complex interplay of mechanical, thermal, and chemical processes in reactive heterogeneous mixtures.

II. ACCOMPLISHMENTS

What follows is a summary of the most important results in each of the two computational model developments. A list of all publications and reports is provided in section III.

1. Continuum VIR model

This model was originally developed to describe unusual chemical reactions observed in NCSU experiments involving a mixture of Ni-Al powders having diameters of a few to tens of micrometers. These experiments showed that high-pressure shock compression of the exothermic mixture released a substantial energy at the shock front in time scales on the order of one microsecond or less that cannot be explained by conventional reaction theories of solid state reactions. Typical chemical reactions in powder mixtures of several micrometers in diameter require the time duration of seconds or longer for completion. In addition, high-pressure is known to decrease the diffusion

rate and reaction products become barriers for the further propagation of chemical reaction.

VIR is an irreversible thermodynamics model aimed at capturing overall features of chemical reactions in mixed powders and its interaction with hydrodynamic flow [16, 17]. It is a simple multi-component, reactive model developed for hydrocode applications. Several important features considered in the original model are (1) explicit effects of porosity, (2) multi-component thermodynamic systems to describe heterogeneous chemical reaction and energy transport between subsystems, (3) effects of energy release by these reactions, (4) effects of changes in specific volume, (5) a single effective chemical reactions, and mechanical equilibrium of the subsystems. The most recent version of the model includes mass transport between the subsystems as well as multi-reactions. It is shown recently [7] that VIR is a generalized form of other well known reaction models: Hermann, Johnson, and Johnson-Tang-Forrest models. The major difference between VIR and the other models is that in the former the second law of thermodynamics plays the central role in the formulation of constitutive behavior.

The predictive capability of the VIR model has been tested for analysis and interpretation of real time response of not only the Ni-Al mixture, but also other mixtures such as Al-Fe₂O₃, Ti-Si, Ti-Teflon, and diamond-Si-C. However, due to the limited scope of the experimental data available at the present time, these calculations were based on hypothesized reactions and idealized estimates of the material constants. Nevertheless, the results show that the model can be made to describe the real time profiles within a reasonable bound of material constants. The significance of the model simulation is not so much the closeness of the agreement obtained between the experiments and the calculations, but the result that the hypothesized reactions must initiate in the shock front and have characteristic time scales of one microsecond or less. Mechanistic understanding of such ultra-fast reactions at the particle level has been the goal of the second phase of this research project.

The most notable application of the VIR model was a comprehensive analysis of condensed phase detonation involving a Ni-Al mixture. This analysis showed numerically for the first time, the possibility of a self-supporting reaction wave in an inorganic solid-liquid system. There are experimental attempts to demonstrate such a possibility by use of more exothermic systems such as Mn-S and Ti-C. If proven, it will be definitive proof of the above described shock-induced chemical reactions in inorganic powder mixtures.

2. DM2 Modeling

DM2 (or DM²) is an acronym of the computational code called Discrete Meso-Dynamic Method in two spatial dimensions. The genesis of this code was a joint research project in 1994 between NCSU and the Russian Materials Center, Tomsk, Russia, that was funded in part by US Army research Office, Sandia National Laboratories, and North Carolina Super Computer Center. The primary purpose of this code is to develop a new computational technique for modeling the response of granular and heterogeneous materials to high rates of loading at the particle level. But, it has now been tested for other materials as well as quasi-static loading.

DM2 is basically a quasi-molecular code in which macroscopic materials are represented by a collection of discretized, particulate elements. The fundamentals of this code are detailed in [8]. In contrast to other discrete element codes, DM2 is a multi-physics code and is capable of describing mechanical, thermal, and chemical interactions between elements. The mechanical interactions are based on the classical equations of motion involving such contact forces as radial potential force, viscous damping force, shear resistance, and friction. The selection of these forces depends on the nature of the problem under investigation.

In DM2, material geometry that may contain inhomogeneity and anisotropy can be created by selective assignment of not only material properties, but also bonding and contact states of individual elements as well as areas of materials discontinuities. Elements also have

internal state parameters and can change their phase or composition through chemical reaction with neighboring elements. A change of state or composition is typically controlled by a specification of the prescribed threshold conditions that are a function of temperature and pressure. Thus, the materials response in DM2 is represented by the aggregate evolution of element movement and their internal state.

The code has been used to model a variety of materials that are subjected to both dynamic and quasi-static loading. The following selected list of model calculations that have been conducted so far indicates the scope of the code capability.

- Shock-induced reactions in a Ni-Al powder mixture
- Shock compression of steel powder
- Shock wave profiles in HMX explosive powder
- Shock wave propagation in polycrystalline Cu
- Shock compression of anisotropic hBN+Cu powder
- Chemical reactions in a shear band
- Granular Couette flow
- Response of steel-fiber reinforced concrete to ballistic impact
- Ballistic penetration into a reactive powder mixture
- Spall in a metallic plate
- Tension/compression testing of concrete
- Fiber pull-out in concrete

The goal of the above listed calculations was aimed at elucidating the meso-scale phenomena in anisotropic and/or heterogeneous media under high dynamic loading at the particle level. Most of these calculations have not been performed previously (or have been difficult to conduct without a type code like DM2).

Out of all the calculations we have carried out so far, there emerges one conclusion: at the meso-level (on the order of micrometers), the paradigm of the existing shock compression

processes may need significant modification to take account of heterogeneous effects, anisotropic structure, and non-equilibrium thermodynamic effects. For example, in the calculation of polycrystalline Cu, it is found that there exists a new mode of deformation that may significantly affect our basic understanding of dynamic strength of metallic materials. This deformation has a vortex-like structure and appears to be created by the interaction of non-equilibrium mass flow with local anisotropic microstructure. Also, the analysis of a shear band in mixed powders demonstrated that there is a critical strain rate above which the deformation leads to a classic phenomenon of thermal explosion and that it is not just shock heating that initiates this explosion, but a complex interplay of deformation, mass mixing, and exothermic chemical reaction as well. Lastly, but not least, it is found that shock compression of polycrystalline metals creates a large fluctuating stress field even at the terminal, supposedly equilibrium, state. This raises the possibility of developing a new micromechanical interpretation (or reinterpretation) of the extensive metallurgical data on shock compression of metals in terms of loading and local microstructure at the grain level.

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